

## Molecular collision data for hydrogen plasmas

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Molecular collision processes play an important role in plasma kinetics at the divertor and near-wall region of magnetic confinement fusion plasma experiments [1]. Here the primary plasma constituents are atomic hydrogen and helium, their molecules and ions, which may be in rovibrationally and/or electronically excited states. Hence accurate and detailed collision data involving hydrogen and helium species is of great importance for modeling fusion plasmas and many other technological and astrophysical plasmas.

The *ab initio* convergent close-coupling (CCC) method has been extensively applied to model electron collisions with hydrogen and helium atoms [2, 3]. For these atoms this method has been used to calculate accurate and comprehensive collision data sets, which are available on the LXcat database [4]. The CCC implementation for atoms is a complete scattering theory in the sense that it yields accurate elastic, excitation, and ionization cross sections irrespective of the projectile energy.

Presently state-of-the-art scattering theories are routinely applied to study electron-atom collisions with large-scale close-coupling results available for many atoms, however the situation is very different for electron-molecule collisions. The lack of spherical symmetry in collisions involving molecules makes it particularly difficult to treat the collision dynamics accurately. Typically, electron-molecule calculations include just a few states in the close-coupling expansion and convergence studies are not performed. Even for the simplest molecules, molecular hydrogen and its ion, theoretical results were limited to various perturbative techniques ( $H_2^+$ ) or small size close-coupling calculations ( $H_2$ ).

Recently we extended the CCC method to electron scattering from the hydrogen molecule  $H_2$  [5] and its hot (vibrationally excited) ion  $H_2^+$  [6]. The molecular CCC method is formulated in a single-center coordinate system and utilizes the Born-Oppenheimer approximation of the scattering wave function. Molecular electronic target states are constructed via a diagonalization procedure of the electronic Hamiltonian in a basis constructed from Sturmian (Laguerre) functions. Such a basis consists of configurations built from appropriately symmetry adapted Laguerre functions for each set of terms of the conserved quantum numbers  $(m_t, \pi_t, s_t)$ , where  $m_t$  is the total target angular momentum projection,  $s_t$  is the spin and  $\pi_t$  is the parity. The re-

sulting set of target states provides an accurate representation of the low-lying bound states of the target and a square-integrable representation of the target continuum, which allows the CCC method to model all possible electronically driven reaction channels including ionization. These target states are used to perform a multi-channel expansion of the total scattering wave function and formulate a set of close-coupling equations. Expanding the projectile wave function in partial waves the CCC method solves this set of equations in momentum space for the  $T$ -matrix, with higher partial waves are accounted for using a Born top-up procedure.

Calculations are performed at a fixed inter-nuclear distance  $R$  and the fixed-nuclei  $T$ -matrix elements  $T_{fi}^{\text{FN}}(R)$  and corresponding cross sections  $Q_{fi}^{\text{FN}}(R)$  describing the transition between electronic states “f” and “i” are obtained. Convergence of the calculated cross sections can be easily tested by increasing the size of the Laguerre basis and/or close-coupling expansion.

For  $\text{H}_2^+$  we have performed calculations in the adiabatic-nuclei approximation to model scattering from the vibrational states of the hot molecule [6]. In this approach the cross sections are calculated as

$$Q_{f,iv}^{\text{AN}} = \int R^2 dR |\phi_v(R)|^2 Q_{fi}^{\text{FN}}(R),$$

where  $Q_{f,iv}^{\text{AN}}$  is the adiabatic-nuclei cross section,  $\phi_v$  and  $v$  are the initial vibrational wave function and quantum number respectively. To calculate the integral in the above equation accurately requires the fixed-nuclei cross sections at a (large) number of inter-nuclei distances, which is a computationally expensive task for large close-coupling calculations. Such a large computational task became feasible only recently with the CCC computer code’s capability to take advantage of massively parallel supercomputers.

In Fig. 1 we present the vibrationally resolved cross sections for dissociative excitation (DE) and dissociative ionization (DI) of  $\text{H}_2^+$  for  $v$  ranging from 0 to 9. Both DE and DI cross sections

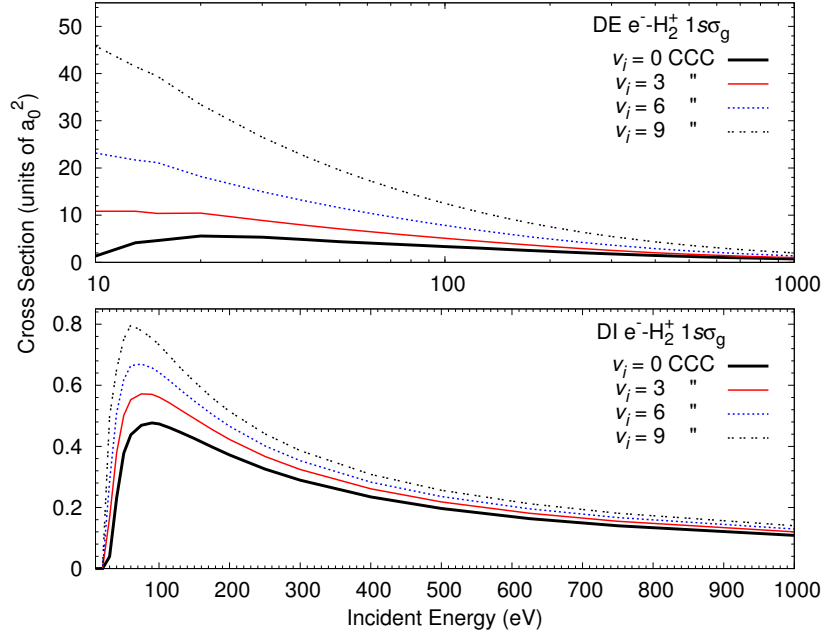


Figure 1: *Dissociative excitation (DE) and dissociative ionization (DI) cross sections for electron scattering from  $\text{H}_2^+$  in the electronic ground, vibrational state  $v_i$ .*

exhibit strong dependence on  $v$  and show significant increase as  $v$  becomes larger. This can be explained by noting that the excitation thresholds become smaller as  $v$  increases. As a function of  $R$  the relative decrease of the thresholds of the two lowest states ( $2p\sigma_u$ ,  $2p\pi_u$ ), which dominate the contribution to DE, is larger than that for ionization. This explains the larger vibrational dependence of the DE cross sections.

Experimentally,  $H_2^+$  ions are produced by ionization of  $H_2$ , which leaves  $H_2^+$  in a distribution of the vibrational levels. Due to the lack of dipole moment of  $H_2^+$  the relaxation of these states via dipole transitions is forbidden and they have long life times. To compare with experiment such a distribution has to be taken into account. The weights associated with the vibrational levels can be taken as the Franck-Condon (FC) distribution or measured in the experiment.

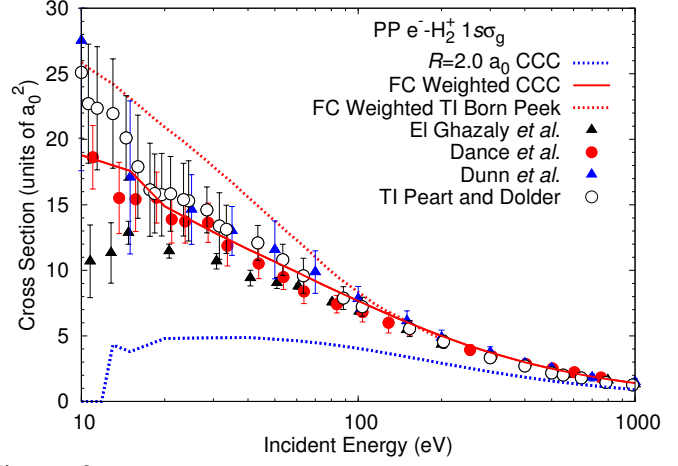


Figure 2: *Vibrationally weighted proton production (PP) cross sections for electron scattering from the electronic ground, vibrationally excited states of  $H_2^+$ .*

In Fig. 2 we present the cross section for proton production (PP)  $Q_{PP} = Q_{DE} + 2Q_{DI}$ . CCC cross sections have been weighted according to the FC distribution and are compared with the present  $R = 2.0 a_0$  fixed-nuclei calculations, total inelastic (TI) Born calculations of Peek [7], the TI measurements of Peart and Dolder [8], and the PP experiments [9-11]. Note that TI cross sections are  $Q_{TI} = Q_{DE} + Q_{DI}$ . Given that  $Q_{DE}$  is much larger than  $Q_{DI}$  the PP and TI cross sections differ insignificantly. By taking into account the vibrationally excited states of the molecule, we observe a strong enhancement of the PP cross section from the fixed-nuclei values. These FC weighted PP cross sections are also in good agreement with experiments, indicating that account of the vibrational distribution is necessary. At high energies our results are in good agreement with the first-order calculations of Peek [7]. Variation in experimental results at low energies is primarily due to the differences in the vibrational distributions of the corresponding experiments.

We now turn to electron scattering from  $H_2$ . We have performed large-scale close-coupling calculations in the fixed-nuclei approximation for incident electron energies from 0.1 to 300 eV [5]. Convergence of the close-coupling expansion was established by increasing the size of the calculations from nine to 491 states. As a demonstration of the method, in Fig. 3 we present the grand total scattering cross section (GTCS) and compare with experimental results [12-19]. To date these are the only *ab initio* results of the GTCS across the intermediate energy region that

are in excellent agreement with all experiments. The small experimental uncertainties suggest that the CCC formalism is correct across the entire energy range, with elastic, excitation, and ionization processes being taken into account accurately.

The LXcat database [4] has a comprehensive data set of CCC collisions cross sections for electron scattering from the vibrationally excited  $\text{H}_2^+$  ion and its isotopologues ( $\text{D}_2^+$ ,  $\text{T}_2^+$ ,  $\text{HD}^+$ ,  $\text{HT}^+$ , and  $\text{DT}^+$ ). It includes vibrationally resolved DE, DI and  $2p\sigma_u$  and  $2p\pi_u$  excitation cross sections. In the near future we are planning to provide a comprehensive data set of e- $\text{H}_2$  cross sections, some of which are already available on the LXcat database.

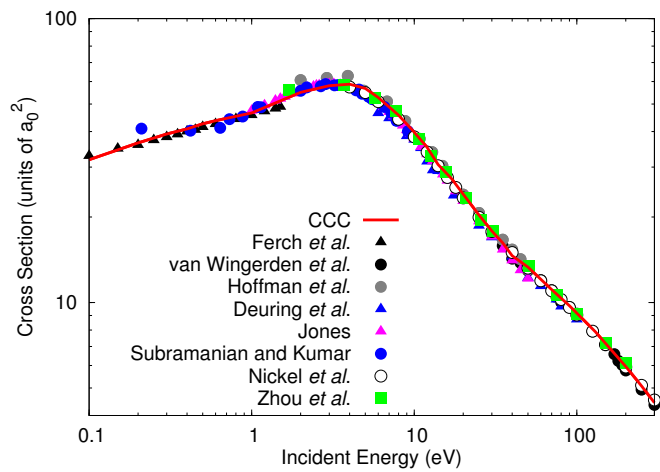


Figure 3: Grand total cross section of electron scattering from the ground state of  $\text{H}_2$ .

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